Chapter 2

Linear Algebra

In this chapter, we study the formal structure that provides the background for quantum mechanics. The basic ideas of the mathematical machinery, linear algebra, are rather simple and learning them will eventually allow us to explain the strange results of spin-half measurements. We start by considering the run of the mill vectors one encounters early in classical physics. We then study matrices and how they can be used to represent vectors and their operators. Finally we briefly look at Dirac's notation, which provides an algebraic scheme for quantum mechanics. This chapter is rather long and complex; however, it contains almost all the math we need for the rest of the book.

2.1. Vectors

Some physical quantities such as mass, temperature, or time are scalar because they can be satisfactorily described by using a magnitude, a single number together with a unit of measure. For example, mass is thoroughly described by stating its magnitude in terms of kilograms. However, other physical quantities such as displacement (change in position) are vectorial because they cannot be satisfactorily described merely by providing a magnitude; one needs to know their direction as well: when one changes position, direction matters. Consider a particle moving on a plane (on this page, for example) from point x to point y. The directed straight-line segment going from x to y is the displacement vector of the particle, and it represents the particle's change in position.

A vector is represented by boldface letters (e.g., \mathbf{A} , \mathbf{b}). The norm or magnitude of vector \mathbf{A} is represented by $|\mathbf{A}|$; it is always positive. Given two vectors \mathbf{A} and \mathbf{B} , their sum $\mathbf{A} + \mathbf{B}$ is obtained by placing the tail of \mathbf{B} on the tip of \mathbf{A} ; the directed segment \mathbf{C}

joining the tail of A to the tip of B is the result of the addition. Equivalently, one can place A and B so that their tails touch and complete the parallelogram of which they constitute two sides. The directed segment C along the diagonal of the parallelogram and whose tail touches those of A and B, is the result of the addition (Fig. 1).

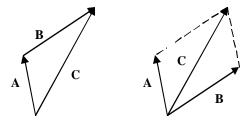


Figure 1

Notice that vector addition is commutative $(\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A})$ and associative $(\mathbf{A} + [\mathbf{B} + \mathbf{C}] = [\mathbf{A} + \mathbf{B}] + \mathbf{C})$.

The negative of \mathbf{A} is the vector with the same magnitude but opposite direction and is denoted by $-\mathbf{A}$. The difference $\mathbf{B} - \mathbf{A}$ is $\mathbf{B} + (-\mathbf{A})$, namely, the sum of \mathbf{B} and the negative of \mathbf{A} . The scalar product of \mathbf{A} by a scalar k is a vector with the same direction as \mathbf{A} and magnitude $k|\mathbf{A}|$, and is designated by $k\mathbf{A}$.

EXAMPLE 2.1.1

Let \mathbf{A} as a 3 meters displacement vector due North and \mathbf{B} a 4 meters displacement vector due East. Then, $\mathbf{A} + \mathbf{B}$ is a 5 meter long vector due North-East; $-\mathbf{A}$ is a 3 meter vector pointing South; $\mathbf{B} - \mathbf{A}$ is a 5 meter vector pointing South-East.

2.2. The Position Vector and its Components

Consider the standard two-dimensional Cartesian grid. The position of a point P can be given by the two coordinates x and y. However, it can also be described by the position vector, a displacement vector \mathbf{r} from the origin to the point.

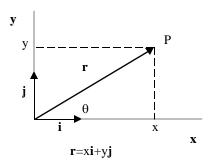


Figure 2

There is an important connection between x, y, and \mathbf{r} . Let us define two unit vectors \mathbf{i} , \mathbf{j} (that is, vectors of magnitude $|\mathbf{i}| = |\mathbf{j}| = 1$) that point in the positive directions of the x and y axis respectively. Then, $\mathbf{r} = x\mathbf{i} + y\mathbf{j}$. For example, if P has coordinates x = 1m, y = 3m, then $\mathbf{r} = 1\mathbf{i} + 3\mathbf{j}$. In addition, a look at figure 3 shows that if \mathbf{A} has components A_x , A_y , and \mathbf{B} has components $B_x B_y$, then $\mathbf{R} = \mathbf{A} + \mathbf{B}$ has components $R_x = A_x + B_x$ and $R_y = A_y + B_y$. So, once we know the components of two vectors, we can determine the components of their sum.

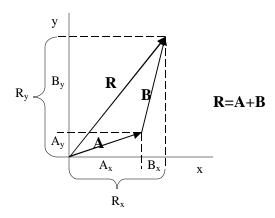


Figure 3

¹ From now on, we shall denote meters with the symbol "m". The extension to three dimensions is immediate. One just adds a new unit vector, \mathbf{k} , perpendicular to the other two.

This can be extended to three dimensions by adding the unit vector \mathbf{k} associated with the z-axis. The dot product of two vectors \mathbf{A} and \mathbf{B} , is the number (a scalar!)

$$\mathbf{A} \bullet \mathbf{B} = a_x b_x + a_y b_y + a_z b_z. \tag{2.2.1}$$

EXAMPLE 2.2.1

Let $\mathbf{r}_1 = 2\mathbf{i} + 3\mathbf{j} + 1\mathbf{k}$ and $\mathbf{r}_2 = 1\mathbf{i} + 2\mathbf{j} + 1\mathbf{k}$.

Then, $\mathbf{r}_1 \bullet \mathbf{r}_2 = 2 + 6 + 1 = 9$.

2.3 Vector Spaces

We are now going to deal with vectors at a more abstract level. In keeping with standard notation, we represent a vector by a letter enclosed in the symbol " $|\rangle$ ", called a "ket." A complex vector space V is a set of vectors $|A\rangle, |B\rangle, |C\rangle$ … together with a set of scalars constituted by complex numbers a,b,c..., and two operations, *vector addition* and *scalar multiplication*.²

Vector addition is characterized by the following properties:

- 1. It is commutative: $|A\rangle + |B\rangle = |B\rangle + |A\rangle$.
- 2. It is associative: $|A\rangle + (|B\rangle + |C\rangle) = (|A\rangle + |B\rangle) + |C\rangle$.
- 3. There exists a null vector $|0\rangle$, usually symbolized simply by 0, such that for every vector $|A\rangle$, $|A\rangle + 0 = |A\rangle$.
- 4. Every vector $|A\rangle$ has an inverse vector $|-A\rangle$ such that $|A\rangle + |-A\rangle = 0$.

 2 i is an imaginary number whose value is $i = \sqrt{-1}$. Algebraically, i is manipulated like an ordinary number, that is, a real number, as long as one remembers that $i^{2} = -1$. A complex number has the form x + yi. For example, 3 is a complex number (x = 3; y = 0), and so are $\pi + 2i$ ($x = \pi; y = 2$), and i (x = 0; y = 1).

Scalar multiplication is characterized by the following properties:

- 1. It is distributive with respect to vector and scalar addition: $a(|A\rangle + |B\rangle) = a|A\rangle + a|B\rangle$ and $(a+b)|A\rangle = a|A\rangle + b|A\rangle$, where a and b are scalars.
- 2. It is associative with respect to multiplication of scalars: $(ab)|A\rangle = a(b|A\rangle)$, where a and b are scalars.
- 3. $0|A\rangle = |0\rangle$: any vector times 0 is the null vector; $1|A\rangle = |A\rangle$: any vector times 1 is the same vector; $-1|A\rangle = |-A\rangle$: any vector times -1 is the inverse of the vector.

In short, addition and scalar multiplication of two vectors follow the usual algebraic rules for addition and multiplication.

We now introduce some important definitions. A linear combination of vectors $|A\rangle, |B\rangle, |C\rangle$..., has the form $c_1|A\rangle + c_2|B\rangle + c_3|C\rangle + ...$ For example, any vector in the *xy*-plane can be expressed as a linear combination of the unit vectors \mathbf{i} and \mathbf{j} . A vector $|X\rangle$ is linearly independent of the set $|A\rangle, |B\rangle, |C\rangle$..., if it cannot be expressed as a linear combination of them. For example, in three dimensions the unit vector \mathbf{k} is linearly independent of the set \mathbf{i}, \mathbf{j} . By extension, a set of vectors is linearly independent if each vector is linearly independent of all the others.

A set of vectors is complete (or spans the space) if every vector in that space can be expressed as a linear combination of the members of the set. For example, the set of vectors **i**, **j** spans the space of vectors in the *xy*-plane but not the space of vectors in the

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³ We keep representing the unit vectors of standard Cartesian coordinates as we did earlier, namely as i,j,k.

xyz-plane. A linearly independent set of vectors that spans the space is a *basis* for the space, and the number of vectors in a basis is the dimension of the space. For example, the set {i, j,k} is a basis for the vector space constituted by all the vectors in three-dimensional coordinates. Given a space V *and* a basis for it, any vector in V has a unique representation as a linear combination of the vector elements of that basis.

2.4 Matrices

A matrix of order $m \times n$ is a rectangular array of numbers a_{jk} having m rows and n columns. It can be represented in the form

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn} \end{pmatrix}$$

Each number a_{jk} in the matrix is an element; the subscripts j and k indicate the element's row and column, respectively. A matrix with only one row is a row matrix; one with only one column is a column matrix. A square matrix is one having as many rows as columns (m = n). A matrix whose elements are all real numbers is real; a matrix having at least one complex number as an element is complex. Two matrices are of the same order when they have equal numbers of rows and columns. Two matrices are identical when they have exactly the same elements.

We can now define some operations on matrices and some matrices with properties of interest to us. At times, these definitions may seem confusing. However, a look at the examples should clarify matters quite a bit: often, when it comes to matrices there is less than meets the eye.

If A and B are matrices of the *same order* $m \times n$, then the sum A+B is the matrix of order $m \times n$ whose element c_{jk} is the sum of A's element a_{jk} and B's element b_{jk} . Subtraction is defined analogously.

Commutative and associative laws are satisfied:

$$A + B = B + A \tag{2.4.1}$$

and

$$A + (B + C) = (A + B) + C. (2.4.2)$$

If A is a matrix with generic element a_{jk} and λ any number, then the product λA is the matrix whose generic element is λa_{jk} .

The associative law is satisfied:

$$ab(A) = a(bA). (2.4.3)$$

Distributive laws with respect to matrix and scalar addition are also satisfied:

$$a(A+B) = aA + aB, \qquad (2.4.4)$$

and

$$(a+b)A = aA + bA. (2.4.5)$$

EXAMPLE 2.4.1

Let
$$A = \begin{pmatrix} 2 & -3 \\ 1 & 5 \\ 7 & i \end{pmatrix}$$
 and $B = \begin{pmatrix} 4 & -i \\ 2 & 4 \\ -7 & 4 \end{pmatrix}$. Then,

$$A + B = \begin{pmatrix} 6 & -3 - i \\ 3 & 9 \\ 0 & 4 + i \end{pmatrix}; A - B = \begin{pmatrix} -2 & -3 + i \\ -1 & 1 \\ 14 & i - 4 \end{pmatrix}; 2A = \begin{pmatrix} 4 & -6 \\ 2 & 10 \\ 14 & 2i \end{pmatrix}; iB = \begin{pmatrix} 4i & 1 \\ 2i & 4i \\ -7i & 4i \end{pmatrix}.$$

Let A be a $m \times n$ matrix of generic element a_{jk} and B be a $n \times p$ matrix of generic element b_{jk} ; then, the product AB is the matrix C of order $m \times p$ and generic element

$$c_{jk} = \sum_{l=1}^{n} a_{jl} b_{lk} .^{4}$$
 (2.4.6)

EXAMPLE 2.4.2

Let
$$A = \begin{pmatrix} 4 & 2 \\ -3 & 1 \end{pmatrix}$$
, and $B = \begin{pmatrix} 1 & 5 & 3 \\ 2 & 7 & -4 \end{pmatrix}$. Then,

$$AB = \begin{pmatrix} 4 \cdot 1 + 2 \cdot 2 & 4 \cdot 5 + 2 \cdot 7 & 4 \cdot 3 + 2 \cdot (-4) \\ -3 \cdot 1 + 1 \cdot 2 & -3 \cdot 5 + 1 \cdot 7 & -3 \cdot 3 + 1(-4) \end{pmatrix} = \begin{pmatrix} 8 & 34 & 4 \\ -1 & -8 & -13 \end{pmatrix}.$$

Note that AB is defined *only if* the number of columns of A is the same as the number of rows of B (the horizontal span of A is the same as the vertical span of B) that is, if A is conformable with B. ⁵

⁴ \sum is the symbol for summation; its subscript and superscript provide the lower and higher limit. For example, $\sum_{n=1}^{4} n = 1 + 2 + 3 + 4 = 10$ and $\sum_{i=1}^{n} x_i = x_1 + ... + x_n$. When the limits depend on the context, it is easier to use the notation $\sum_{i=1}^{n} i$. (2.4.6) looks daunting, but example 2.4.2 should clarify things. Note also that here i is used as an index, not as an imaginary number.

⁵ Note that if *A* is conformable with *B*, it does not follow that *B* is conformable with *A*. For example, $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is conformable with $B = \begin{pmatrix} e \\ f \end{pmatrix}$ because *A*'s horizontal span (2 elements) is the same as *B*'s vertical span. However, the converse is not true: *B* is not

Associative and distributive laws with respect to matrix addition and subtraction are satisfied:

$$A(BC) = (AB)C \tag{2.4.7}$$

and

$$A(B \pm C) = AB \pm AC \text{ and } (B \pm C)A = BA \pm CA.$$
 (2.4.8)

However, very importantly, it is *not* always the case that *AB*=*BA*, that is, matrix multiplication is not commutative. The difference between the two products is the *commutator*:

$$AB - BA = [A, B]. \tag{2.4.9}$$

So, although it may happen that [A,B] = 0, this equality cannot be assumed.⁶

If a matrix is square (it has an identical number of rows and columns), then it can be multiplied by itself; it is customary to write AA as A^2 , etc.

EXAMPLE 2.4.3

Let
$$A = \begin{pmatrix} 2 & i \\ 4 & 3 \end{pmatrix}$$
 and $B = \begin{pmatrix} i & 1 \\ 2 & -4 \end{pmatrix}$. Then,

$$AB = \begin{pmatrix} 2i + 2i & 2 - 4i \\ 4i + 6 & -8 \end{pmatrix}; \ BA = \begin{pmatrix} 2i + 4 & +2 \\ -12 & 2i - 12 \end{pmatrix}; \ \begin{bmatrix} A,B \end{bmatrix} = \begin{pmatrix} 2i - 4 & -4i \\ 4i + 18 & -2i + 4 \end{pmatrix}.$$

Notice that in this case $AB \neq BA$.

conformable with A. The matrix multiplication we have just considered is also called the *Cayley product*. There are other types of matrix multiplication. Later, we shall deal with the tensorial (or Kroneker) product of matrices.

⁶ O is the matrix whose elements are all zeros.

If the rows and columns of a matrix A are interchanged, the resulting matrix \tilde{A} is the transpose of A. A square matrix A is symmetric if it is equal to its transpose, $A = \tilde{A}$. In other words, A is symmetric if reflection on the main diagonal (upper left to lower right) leaves it unchanged.

EXAMPLE 2.4.4

Let
$$A = \begin{pmatrix} 1 & 3 \\ 2i & 4 \\ 1 & 0 \end{pmatrix}$$
; then $\tilde{A} = \begin{pmatrix} 1 & 2i & 1 \\ 3 & 4 & 0 \end{pmatrix}$.

$$A = \begin{pmatrix} i & 3 \\ 3 & 5 \end{pmatrix} \text{ and } B = \begin{pmatrix} 1 & 2 & -i \\ 2 & 3 & 1 \\ -i & 1 & 4 \end{pmatrix} \text{ are symmetric.}$$

If all the elements of a matrix A are replaced by their complex conjugates, then A^* is A's complex conjugate. ⁷

The complex conjugate of the transpose of a matrix A is A^+ , A's adjoint. A square matrix A that is identical to the complex conjugate of its transpose (its adjoint), that is, such that $A = \tilde{A}^* = A^+$, is *Hermitian* or *self-adjoint*. As we shall see, Hermitian matrices play a central role in quantum mechanics. A square matrix I with ones in the main diagonal and zeros everywhere else is a unit matrix. Note that given any matrix A, AI = IA = A. (2.4.10)

Finally, the trace Tr(A) of a (square) matrix A is the sum of the elements of the main diagonal. Importantly, we should note that

⁷ Given an expression a, a^* is obtained by changing the sign of all the symbols i in a and leaving the rest untouched. For example, if a = 3i + 2x, then $a^* = -3i + 2x$.

$$Tr(A+B) = Tr(A) + Tr(B),$$
 (2.4.11)

(the trace of a sum of matrices is equal to the sum of the traces of those very same matrices) and

$$Tr(aA) = aTr(A).$$
⁸ (2.4.12)

EXAMPLE 12.4.6

Let
$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
; then, $\tilde{A} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$, and $\tilde{A}^* = A^+ = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Hence, A is Hermitian;

moreover,
$$Tr(A) = 0 + 0 = 0$$
. In addition, $Tr\begin{pmatrix} 1 & 2 & 1 \\ 3 & 2 & 2 \\ 1 & 1 & 4 \end{pmatrix} = 1 + 2 + 4 = 7$.

2.5 Vectors and Matrices

Suppose now that we have a vector space with a given basis $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$.

Then, any vector $|A\rangle$ in the space can be expressed as a linear combination of the basis vectors:

$$|A\rangle = c_1|e_1\rangle + c_2|e_2\rangle + \dots c_n|e_n\rangle, \tag{2.5.1}$$

or more simply

$$|A\rangle = \sum_{i} c_{i} |e_{i}\rangle. \tag{2.5.2}$$

Hence, any vector $|A\rangle$ can be represented as a column matrix

$$\begin{pmatrix} c_1 \\ c_2 \\ \dots \\ c_n \end{pmatrix}$$

where the c_i 's are the expansion coefficients of $|A\rangle$ into the basis $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$.

⁸ Because of (2.4.11) and (2.4.12), the operation of taking the trace is *linear*.

For example, consider vector $|A\rangle = 2\mathbf{i} + 6\mathbf{j} + 0\mathbf{k}$ in three-dimensional coordinates. Then, the expansion coefficients are 2, 6, and 0, and we can represent the vector as the column matrix

$$|A\rangle = \begin{pmatrix} 2 \\ 6 \\ 0 \end{pmatrix}$$

as long as we remember that 2 is associated with \mathbf{i} , 6 with \mathbf{j} , and 0 with \mathbf{k} . In this way, we can represent any of the basis vectors $|e_i\rangle$ by a string of zeros and a 1 in the i^{th} position of the column matrix. For example,

$$\mathbf{j} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

because $\mathbf{j} = 0\mathbf{i} + 1\mathbf{j} + 0\mathbf{k}$. We can express the sum of two vectors as the sum of the two column matrices representing them and the multiplication of a vector by a scalar as the scalar product of the column matrix representing the vector and the scalar. The null vector 0 is represented as a column matrix of zeros. In short, once a basis of a vector space is specified (and only then!), we can treat vectors as column matrices.

2.6 Inner Product Spaces and Orthonormal Bases

The inner product $\langle A | B \rangle$ of two vectors $|A\rangle$ and $|B\rangle$ is the generalization of the dot product we have already encountered: it is the complex number

$$\langle A | B \rangle = a_1^* b_1 + a_2^* b_2 + \dots a_n^* b_n = \sum_i a_i^* b_i,$$
 (2.6.1)

where a_i^* is the complex conjugate of a_i , the generic expansion coefficient of $|A\rangle$ and b_i is the generic expansion coefficient of $|B\rangle$. The inner product can easily be shown to satisfy the following three properties:

- 1. Switching the arguments results in the complex conjugate of the original inner product: $\langle A | B \rangle = \langle B | A \rangle^*$.
- 2. The inner product of a vector with itself is always positive: $\langle A \mid A \rangle \ge 0$. Moreover, $\langle A \mid A \rangle = 0$ just in case $|A\rangle = 0$.
- 3. The inner product is linear in the second argument and antilinear in the first:

$$\langle A | bB + cC \rangle = b \langle A | B \rangle + c \langle A | C \rangle$$
 and $\langle aA + bB | cC \rangle = a^* \langle A | C \rangle + b^* \langle B | C \rangle$.

A vector space with inner product is an inner product space.

The norm of a vector $|A\rangle$ is

$$||A\rangle| = \sqrt{\langle A | A \rangle}, \qquad (2.6.2)$$

and it expresses the length of the vector. A vector of norm 1 is a normalized vector. To normalize a vector, we just divide it by its norm, so that normalized $|A\rangle$ is

$$\frac{|A\rangle}{\sqrt{\langle A | A \rangle}}. (2.6.3)$$

For example, suppose that in figure 2 $\mathbf{r} = 4\mathbf{i} + 3\mathbf{j}$. Then, \mathbf{r} 's norm is $\sqrt{4 \cdot 4 + 3 \cdot 3} = 5$, and once normalized, $\mathbf{r} = \frac{4}{5}\mathbf{i} + \frac{3}{5}\mathbf{j}$. Two vectors whose inner product is zero are orthogonal (perpendicular). A basis of mutually orthogonal and normalized vectors is an orthonormal basis. For example, the set $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ is an orthonormal basis for the vector space of Cartesian coordinates. The component a_i of a vector $|A\rangle$ can be easily obtained using (2.6.1):

⁹ Note that since $|x|^2 = x^* \cdot x$, $\langle A | A \rangle = |a_1|^2 + |a_2|^2 + ... + |a_n|^2$.

¹⁰ From now on, we shall always work with orthonormal bases.

$$\langle \mathbf{e}_i \mid \mathbf{A} \rangle = 0a_1 + ... + 1a_i + ... + 0a_n = a_i,$$
 (2.6.4)

where $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$ is the orthonormal basis. Notice that all this machinery is nothing but a generalization of the characteristics of the more familiar vector space in Cartesian coordinates with $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ as orthonormal basis.

2.7 Linear Operators, Matrices, and Eigenvectors

An operator is an entity that turns vectors in a vector space into other vectors in that space by, say, lengthening them, shortening them, or rotating them. The operator \hat{T} is linear just in case it satisfies two conditions:

1.
$$\hat{T}(|A\rangle + |B\rangle) = \hat{T}|A\rangle + \hat{T}|B\rangle$$
 (2.7.1)

2.
$$\hat{T}(b|A\rangle) = b\hat{T}|A\rangle$$
. (2.7.2)

As one might expect, if we know what a linear operator \hat{T} does to the basis vectors $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$, we can determine what it will do to all the other vectors in the vector space V. It turns out that if \hat{T} is a linear operator, given a basis, \hat{T} can be expressed as a $n \times n$ (square) matrix

$$\hat{T} = \begin{pmatrix} T_{11} & \dots & T_{1n} \\ \dots & \dots & \dots \\ T_{n1} & \dots & T_{nn} \end{pmatrix}, \tag{2.7.3}$$

where n is the dimension of V, and

$$T_{ij} = \left\langle e_i \middle| \hat{T} e_j \right\rangle. \tag{2.7.4}$$

In addition, \hat{T} 's operation on a vector

$$|A\rangle = \begin{pmatrix} a_1 \\ \dots \\ a_n \end{pmatrix} \tag{2.7.5}$$

is nothing but the product of the two matrices:

$$\hat{T}|A\rangle = \begin{pmatrix} T_{11} & \dots & T_{1n} \\ \dots & \dots & \dots \\ T_{n1} & \dots & T_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ \dots \\ a_n \end{pmatrix}.$$
(2.7.6)

So, given a basis, linear operations on vectors can be expressed as matrices multiplying other matrices.

We are going to be interested in particular types of linear operators, namely, those which transform vectors into multiples of themselves:

$$\hat{T}|A\rangle = \lambda |A\rangle,\tag{2.7.7}$$

where λ is a complex number. In (2.7.7), $|A\rangle$ is an eigenvector and λ the eigenvalue of \hat{T} with respect to $|A\rangle$.¹¹ Obviously, given any vector, there are (trivially) an operator and a scalar satisfying (2.7.7). However, in a complex vector space (a vector space where scalars are complex numbers) every linear operator has eigenvectors and corresponding eigenvalues, and, as we shall soon see, some of these are physically significant.¹² Notice that given a basis $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$, if $\hat{T}e_j = \lambda e_j$ (the basis vectors are eigenvectors of \hat{T}), then (2.7.4) and the fact that $\langle e_i|e_j\rangle=0$ unless i=j, guarantee that $T_{ij}=0$ unless i=j. Moreover, given (2.7.4), and the fact that $\langle e_i|\lambda_i e_i\rangle=\lambda_i$, in the basis $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$ all

It is worth noting that eigenvector equations, equations like (2.7.7), are basis-invariant: changing the basis does not affect them at all; in particular, the eigenvalues remain the same.

¹² This is not true in a real vector space (one in which all the scalars are real numbers). Although there are procedures for determining the eigenvalues and eigenvectors of an operator, we shall not consider them here.

the elements in the matrix representing \hat{T} will be zero with the exception of those in the main diagonal (from top left to bottom right), which is constituted by the eigenvalues:

$$\hat{T} = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \lambda_n \end{bmatrix}.$$
 (2.7.8)

A matrix with this form is *diagonalized* in the basis $\{|e_1\rangle, |e_2\rangle, ... |e_n\rangle\}$, and in that basis its eigenvectors look quite simple:

$$|e_{\lambda=1}\rangle = \begin{pmatrix} 1\\0\\...\\0 \end{pmatrix}; |e_{\lambda=2}\rangle = \begin{pmatrix} 0\\1\\...\\0 \end{pmatrix}; ...; |e_{\lambda=n}\rangle = \begin{pmatrix} 0\\0\\...\\1 \end{pmatrix}. \tag{2.7.9}$$

2.8 Hermitian Operators

As we know, a Hermitian matrix is identical to the complex conjugate of its transpose: $A = A^+$. Given an orthonormal basis, the linear operator corresponding to an Hermitian matrix is an Hermitian operator \hat{T} . More generally, an Hermitian operator can be defined as the operator which, when applied to the second member of an inner product, gives the same result as if it had been applied to the first member:

$$\langle \mathbf{A} | \hat{T} \mathbf{B} \rangle = \langle \hat{T} \mathbf{A} | \mathbf{B} \rangle.$$
 (2.8.1)

Hermitian operators have three properties of crucial importance to quantum mechanics that we state without proof:

1. The eigenvalues of a Hermitian operator are real numbers. 13

13 The converse is not true: some operators with real eigenvalues are not Hermitian.

- 2. The eigenvectors of a Hermitian operator associated with distinct eigenvalues are orthogonal.
- 3. The eigenvectors of a Hermitian operator span the space.¹⁴

So, we can use the eigenvectors of a Hermitian operator as a basis, and as a result the matrix corresponding to the operator is diagonalizable.

EXAMPLE 2.8.1

Let us show that $T = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}$ is Hermitian and satisfies (1)-(3). We start by noticing

that

$$T^{+} = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix} = T, \tag{2.8.2}$$

so that *T* is Hermitian.

Given $T|X\rangle = \lambda |X\rangle$, we obtain

$$\begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \tag{2.8.3}$$

or

$$\begin{pmatrix} x_1 + x_2(1-i) \\ x_1(1+i) + 0 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$
 (2.8.4)

Since two matrices are equal just in case they have equal elements, (2.8.3) reduces to a system of two simultaneous equations

¹⁴ This property always holds for finite-dimensional spaces but not always for infinite-dimensional spaces. Since, as we shall see, quantum mechanics involves an infinite vector space (the Hilbert space), this presents some complications we need not consider.

$$\begin{cases} (1-\lambda)x_1 + (1-i)x_2 = 0\\ (1+i)x_1 - \lambda x_2 = 0 \end{cases}, \tag{2.8.5}$$

which has non-trivial solutions (solutions different from zero) just in case its determinant is zero. ¹⁵ We obtain then

$$0 = \begin{vmatrix} 1 - \lambda & 1 - i \\ 1 + i & 0 - \lambda \end{vmatrix} = -\lambda(1 - \lambda) - (1 - i)(1 + i) = \lambda^2 - \lambda - 2 = 0,$$
 (2.8.6)

which has two solutions $\lambda_1 = -1$ and $\lambda_2 = 2$. Hence, the eigenvalues are real numbers.

To obtain the eigenvectors, we plug $\lambda_1 = -1$ into (2.8.5) and obtain

$$\begin{cases} x_1 + x_2(1-i) = -x_1 \\ x_1(1+i) = -x_2 \end{cases}$$
 (2.8.7)

The second equation of (2.8.7) gives us

$$x_2 = (-1 - i)x_1, (2.8.8)$$

so that denoting the eigenvector associated to $\lambda_1 = -1$ with $|X_{\lambda=-1}\rangle$, we obtain

$$\left|X_{\lambda=-1}\right\rangle = x_1 \begin{pmatrix} 1 \\ -1-i \end{pmatrix}. \tag{2.8.9}$$

By an analogous procedure for $\lambda_2 = 2$, we obtain

$$(1+i)x_1 = 2x_2, (2.8.10)$$

that is

$$\left|X_{\lambda=2}\right\rangle = x_1 \left(\frac{1}{1+i}\right) = x_1 \frac{1}{2} \left(\frac{2}{1+i}\right).$$
 (2.8.11)

We can now easily verify that these two eigenvectors are orthogonal. For,

$$\langle X_{\lambda=-1} | X_{\lambda=2} \rangle = (1^*)(2) + (-1-i)^*(1+i) = 2 + (i^2-1) = 2 - 2 = 0.$$
 (2.8.12)

¹⁵ A determinant $\begin{vmatrix} a & b \\ c & d \end{vmatrix}$ is just the number ad - bc.

Let us now normalize the two eigenvectors. The norm of $\left|X_{_{\lambda=-1}}\right\rangle$ is

$$\sqrt{|1|^2 + |-1 - i|^2} = \sqrt{1 + (-1 - i)^* (-1 - i)} = \sqrt{1 + (-1 + i)(-1 - i)} = \sqrt{1 + (1 - i)^2} = \sqrt{1 + 2} = \sqrt{3}.$$
(2.8.13)

So, after normalization $|X_{\lambda=-1}\rangle$ becomes $x_1 \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1-i \end{pmatrix}$. The norm of $|X_{\lambda=2}\rangle$ is

$$\sqrt{1 + \frac{1+i}{2} \frac{1-i}{2}} = \sqrt{\frac{6}{4}} = \frac{\sqrt{6}}{2}.$$
 (2.8.14)

Hence, after normalization
$$|\mathbf{X}_{\lambda=2}\rangle$$
 becomes $x_1 \frac{2}{\sqrt{6}} \left(\frac{1}{1+i}\right) = x_1 \frac{1}{\sqrt{6}} {2 \choose 1+i}$.

2.9 Dirac Notation

If vectors $|A\rangle$ and $|B\rangle$ are members of a vector space V, the notation for their inner product is $\langle A|B\rangle$. In Dirac notation, one may separate $\langle A|B\rangle$ into two parts $\langle A|$, called a bra-vector (bra for short), and $|B\rangle$, called a ket-vector (ket for short). $\langle A|$ may be understood as a linear function that when applied to $|B\rangle$ yields the complex number $\langle A|B\rangle$. The collection of all the bras is also a vector space, the dual space of V, usually symbolized as V^* . It turns out that for every ket $|A\rangle$ there is a bra $\langle A|$ associated with it and within certain constraints that need not concern us the converse is true as well. In addition, a ket and its associated bra are the transpose complex conjugate of each other. So, for example, if $|A\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$, then $\langle A| = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix}$. Note that as $\langle A|B\rangle$ is a number, so $|A\rangle\langle B|$ is an operator. To see why, let us apply $|A\rangle\langle B|$ to a vector $|C\rangle$ to obtain $|A\rangle\langle B|C\rangle$; since $\langle B|C\rangle$ is a scalar c and $c|A\rangle\langle B|$ is a vector, when applied to vector $|C\rangle$, $|A\rangle\langle B|$ yields a vector, and therefore $|A\rangle\langle B|$ is an operator.

When handling Dirac notation, one must remember that order is important; as we saw, $\langle A|B\rangle$ is a scalar, but $|B\rangle\langle A|$ is an operator. The following rules, where c is a scalar, make things easier:

$$\langle A|B\rangle^* = \langle B|A\rangle,\tag{2.9.1}$$

$$\langle A|cB\rangle = c\langle A|B\rangle,$$
 (2.9.2)

$$\langle cA|B\rangle = c^*\langle A|B\rangle,$$
 (2.9.3)

$$\langle A + B | C + D \rangle = \langle A | C \rangle + \langle A | D \rangle + \langle B | C \rangle + \langle B | D \rangle. \tag{2.9.4}$$

Scalars may be moved about at will, as long as one remembers that when they are taken out of a bra, we must use their complex conjugates, as in (2.9.3).¹⁶

Any expression can be turned into its complex conjugate by replacing scalars with their complex conjugates, bras with kets, kets with bras, operators with their adjoints, and finally by reversing the order of the factors. For example,

$$\left\{ \langle \psi | \hat{O} | \gamma \rangle | A \rangle \langle B | c \right\}^* = c^* | B \rangle \langle A | \langle \gamma | \hat{O}^+ | \psi \rangle, \tag{2.9.5}$$

where \hat{O}^+ is the adjoint of \hat{O}^{17} .

Finally, if
$$|A\rangle = \sum_{i} c_{i} |e_{i}\rangle$$
, as per (2.5.2), then

$$c_i = \langle e_i | A \rangle, \tag{2.9.6}$$

for

$$\langle e_i | A \rangle = 0c_1 + \dots + 1c_1 + \dots + 0c_n = c_1.$$
 (2.9.7)

¹⁶ Dirac notes: "We have now a complete algebraic scheme involving three kinds of quantities, bra vectors, ket vectors, and linear operators." (Dirac, P., (1958), 25). Dirac notation proves powerful indeed, as we shall see.

¹⁷ The expression $\langle \psi | \hat{O} | \gamma \rangle$ merely tells us first to apply the operator \hat{O} to $| \gamma \rangle$, thus obtaining a new vector $| \chi \rangle$ and then to obtain the inner product $\langle \psi | \chi \rangle$.

In other words, in order to obtain the expansion coefficient associated with the basis vector $|e_i\rangle$ in the expansion of a vector $|A\rangle$, one takes the bra of $|e_i\rangle$ and multiplies it by $|A\rangle$ or, which is the same, one computes the inner product $\langle e_i|A\rangle$.

Exercises

Exercise 2.1

- 1. True or false: The set $\{i, j, 2i + j\}$ is complete, that is, it spans ordinary three-dimensional space.
- 2. True or false: The set $\{i, j, 2i + j\}$ is linearly independent.
- 3. True or false: The set $\{i, j, 2i + j\}$ is a basis for the xy-plane.
- 4. True or false: A vector space has only one basis.

Exercise 2.2

- 1. Let $A = \begin{pmatrix} 1 & 0 & i \\ 2 & 3 & 0 \end{pmatrix}$; $B = \begin{pmatrix} i & 2 & 1 \\ 3 & 2i & 0 \end{pmatrix}$. Determine: a. A + B; b. A B; c. [A, B].
- 2. Let $A = \begin{pmatrix} 2i & 3 \\ 1 & 0 \end{pmatrix}$; $B = \begin{pmatrix} -i \\ 2 \end{pmatrix}$. Determine: a. A + B; b. A B; c. AB. Is BA defined?
- 3. Let $A = \begin{pmatrix} 3 & -i \\ i & 0 \end{pmatrix}$; $B = \begin{pmatrix} i & 2 \\ 0 & -i \end{pmatrix}$. Determine: a. A + B; b. A B; c. [A, B]

Exercise 2.3

- 1. Let $A = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$. Determine: a. \tilde{A} and A^+ ; b. Is A Hermitian?
- 2. Let $B = \begin{pmatrix} i & i \\ -i & 2 \end{pmatrix}$. a. Is B Hermitian? b. Determine [A, B], where $\tilde{A} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$.
- 3. Let $C = \begin{pmatrix} 1 & 0 & i \\ 0 & 2 & 0 \\ -i & 0 & 3 \end{pmatrix}$. Is C Hermitian?
- 4. Let $D = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Is D Hermitian?
- 5. Verify that Tr(A+B) = Tr(A) + Tr(B), where $A = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ and $B = \begin{pmatrix} i & i \\ -i & 2 \end{pmatrix}$.

Exercise 2.4

- 1. Let $|A\rangle = (2,i,0,3)$ and $|B\rangle = (0,-i,3i,1)$. a. Determine $\langle A | B \rangle$; b. Verify that $\langle A | B \rangle = \langle B | A \rangle^*$; c. Normalize $|A\rangle$; d. Normalize $|B\rangle$.
- 2. Normalize: a. $|A\rangle = (3,i,-i,1)$; b. $|B\rangle = (0,2,i)$; c. $|C\rangle = (0,0,i)$.
- 3. a. If $|e_i\rangle$ is a basis vector, what is $\langle e_i|e_i\rangle$ equal to? b. If $|A\rangle$ is normalized, what is $\langle A|A\rangle$ equal to? c. If $\langle A|A\rangle=1$ is $|A\rangle$ normalized?

Exercise 2.5

- **1.** Let $\hat{T} = \begin{pmatrix} 0 & 1 & i \\ 2i & 3 & 1 \\ 0 & 3 & -i \end{pmatrix}$ be a linear operator and $|X\rangle = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ a generic vector. Determine $\hat{T}|X\rangle$.
- **2.** Let $\hat{T} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$ and $|X\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$. Determine $\hat{T}|X\rangle$.

Exercise 2.6

Show that $\hat{A} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ is Hermitian. Find its eigenvalues. Then find its eigenvectors,

normalize them, and verify that they are orthogonal.

Exercise 2.7

Determine whether the following statements are true:

a.
$$\langle \psi | O | \phi \rangle | \alpha \rangle c = c | \alpha \rangle \langle \psi | O | \phi \rangle$$
.

b.
$$\langle \psi + \alpha | c \phi \rangle = c (\langle \psi | \phi \rangle + \langle \alpha | \phi \rangle)$$
.

c. $\langle \alpha | O | \phi \rangle | \gamma \rangle \langle \chi |$ is an operator.

Answers to the Exercises

Exercise 2.1

- 1. No. **z** is not expressible as a linear combination of the vectors in the set.
- 2. No. $2\mathbf{i} + \mathbf{j}$ is not independent of the other two vectors in the set.
- 3. No. Although it spans the space, the set is not linearly independent.
- 4. No. For example, ordinary space has an infinity of bases; just rotate the standard basis by any amount to obtain a new basis.

Exercise 2.2

1a:
$$A + B = \begin{pmatrix} 1+i & 2 & 1+i \\ 5 & 3+2i & 0 \end{pmatrix}$$
; 1b: $A - B = \begin{pmatrix} 1-i & -2 & i-1 \\ -1 & 3-2i & 0 \end{pmatrix}$; c: $[A,B]$ is undefined

because A is not conformable with B.

2a: A+B is undefined because A and B are of different order; 2b: A-B is undefined

because A and B are of different order; 2c:
$$AB = \begin{pmatrix} 2+6 \\ -i+0 \end{pmatrix} = \begin{pmatrix} 8 \\ -i \end{pmatrix}$$
; 2d: no, because B is not

conformable with A.

3a:
$$A + B = \begin{pmatrix} 3+i & 2-i \\ i & -i \end{pmatrix}$$
; 3b: $A - B = \begin{pmatrix} 3-i & -2-i \\ i & i \end{pmatrix}$; 3c: $AB = \begin{pmatrix} 3i & 6-1 \\ -1 & 2i \end{pmatrix}$; however,

$$BA = \begin{pmatrix} 3i + 2i & 1 \\ 1 & 0 \end{pmatrix}$$
. Hence, $[A, B] = \begin{pmatrix} -2i & 4 \\ -2 & 2i \end{pmatrix}$.

Exercise 2.3

1a:
$$\tilde{A} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$
; 1b: $\tilde{A}^* = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$; 1c: yes.

2a: No; 2b:
$$AB = \begin{pmatrix} 2i & 2i \\ -2i & 4 \end{pmatrix}$$
; however, $BA = \begin{pmatrix} 2i & 2i \\ -2i & 4 \end{pmatrix}$. Hence, $[A,B] = 0$. In this case the

two matrices do commute!

3a:
$$\tilde{C} = \begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 3 \end{pmatrix} \Rightarrow \tilde{C}^* = \begin{pmatrix} 1 & 0 & i \\ 0 & 2 & 0 \\ -i & 0 & 3 \end{pmatrix}$$
. So, C is Hermitian.

4a: No, because it is not square.

5.
$$A+B=\begin{pmatrix} 2+i & i \\ i & 4 \end{pmatrix}$$
. Hence, $Tr(A+B)=6+i$. But $Tr(A)=4$ and $Tr(B)=2+i$.

Exercise 2.4

1a:
$$\langle A | B \rangle = 2 \cdot 0 + (-i)(-i) + 0 \cdot 3i + 3 \cdot 1 = 2$$
.

1b: $\langle B|A\rangle = 0 \cdot 2 + i \cdot i + (-3i) \cdot 0 + 1 \cdot 3 = 2$. Since, $2^* = 2$, the property is verified.

1c:
$$\langle A \mid A \rangle = 2 \cdot 2 + (-i) \cdot i + 0 \cdot 0 + 3 \cdot 3 = 14$$
. Hence, normalization gives $\frac{1}{\sqrt{14}} \begin{bmatrix} 2 \\ i \\ 0 \\ 3 \end{bmatrix}$.

1d:
$$\langle B | B \rangle = 0 \cdot 0 + i(-i) + (-3i)3i + 1 \cdot 1 = 11$$
. Hence, normalization gives $\frac{1}{\sqrt{11}} \begin{pmatrix} 0 \\ -i \\ 3i \\ 1 \end{pmatrix}$.

2a:
$$\langle \mathbf{A} \mid \mathbf{A} \rangle = 3 \cdot 3 + (-i)i + i \cdot (-i) + 1 \cdot 1 = 12$$
. Hence, normalization gives $\frac{1}{\sqrt{12}} \begin{pmatrix} 3 \\ i \\ -i \\ 1 \end{pmatrix}$.

2b:
$$\langle B | B \rangle = 0 + 4 + 1 = 5$$
. So, normalization gives $\frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ 2 \\ i \end{pmatrix}$.

2c: $\langle C | C \rangle = 0 + 0 + (-i)i = 1$. So, the vector is already normalized.

3a: It is equal to 1, since all the members of the matrix vector representing $|e_i\rangle$ are zero, with the exception of the i^{th} member, which is 1.

3b: It is equal to 1.

3c: Yes.

Exercise 2.5

$$1.\,\hat{T}|X\rangle = \begin{pmatrix} x_2 + ix_3 \\ 2ix_1 + 3x_2 + x_3 \\ 3x_2 + -ix_3 \end{pmatrix}.$$

$$2. \hat{T}|X\rangle = i \begin{pmatrix} x_2 \\ x_1 \end{pmatrix}.$$

Exercise 2.6

 $A = \tilde{A}^* = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and therefore A is Hermitian. The generic eigenvector equations are

$$A|X\rangle = \lambda |X\rangle \Rightarrow \begin{pmatrix} -i\frac{\hbar}{2}x_2 \\ i\frac{\hbar}{2}x_1 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \Rightarrow \begin{cases} \lambda x_1 + i\frac{\hbar}{2}x_2 = 0 \\ i\frac{\hbar}{2}x_1 - \lambda x_2 = 0 \end{cases}. \text{ Hence,}$$

$$0 = \begin{bmatrix} \lambda & i\frac{\hbar}{2} \\ i\frac{\hbar}{2} & -\lambda \end{bmatrix} = -\lambda^2 + \left(\frac{\hbar}{2}\right) \Rightarrow \lambda_{1,2} = \pm\frac{\hbar}{2}.$$
 Consequently, the two eigenvalues are $\lambda_1 = -\frac{\hbar}{2}$

and $\lambda_2 = \hbar/2$. Now, for $\lambda_1 = -\frac{\hbar}{2}$ we obtain $x_1 = ix_2$, and consequently, $|X_{\lambda_1}\rangle = x_2 \binom{i}{1}$.

Since $\langle X_{\lambda_1} | X_{\lambda_1} \rangle = -i \cdot i + 1 = 2$, normalization yields $\frac{1}{\sqrt{2}} \binom{i}{1}$.

For $\lambda_2 = \hbar/2$ we obtain $x_1 = -ix_2$, and consequently $\left| \mathbf{X}_{\lambda_2} \right\rangle = x_2 \begin{pmatrix} 1 \\ i \end{pmatrix}$.

Since $\langle X_{\lambda_2} | X_{\lambda_2} \rangle = i \cdot (-i) + 1 = 2$, normalization yields $\frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}$.

Moreover, $\langle X_{\lambda_1} | X_{\lambda_2} \rangle = -i \cdot -i + 1 \cdot 1 = -1 + 1 = 0$, and consequently the two vectors are orthogonal.

Exercise 2.7

a: Yes; b: Yes; c: Yes.